

Vibrational decoherence in ion-trap quantum computers *

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Abstract

Decoherence is studied in an attractive proposal for an actual implementation of a quantum computer based on trapped ions. Emphasis is placed on the decoherence arising from the vibrational motion of the ions, which is compared with that due to spontaneous emission from excited states of the ions. The calculation is made tractable by exploiting the vast difference in time scales between the vibrational excitations and the intra-ionic electronic excitations. Since the latter are several orders of magnitude faster, an adiabatic approximation is used to integrate them out and find the inclusive probability $P(t)$ for the electronic state of the ions to evolve as it would in the absence of vibrational coupling, and the ions to evolve into any state whatsoever. The decoherence time is found at zero temperature and for any number of ions N in the computer. Comparison is made with the spontaneous emission decoherence, and the implications for how trap voltages and other parameters should be scaled with N are discussed.

1 INTRODUCTION

A quantum computer (QC) is a proposed machine that would make use of the superposition principle of quantum mechanics to do certain types of calculations with an unprecedented degree of parallelism. The concept of a quantum computer goes back to the early 1980's.[1, 2] It is an outgrowth of the view that any computation is ultimately a physical process. This view has tended to get obscured in recent times, especially as our understanding of the universal mathematical properties of computation and associated issues in complexity and computational theory has grown. If one thinks about the computer as a machine, however, in which wheels must turn, or electrons must be transported between transisitors, and so on, then it is somewhat surprising, at least in hindsight, that it has taken us so long to start thinking about the implications of the laws of quantum mechanics for the turning of the wheels, transport of charges etc. To avoid misunderstanding it should be emphasized that quantum mechanics already plays a vital role in the functioning of all modern electronic circuitry, in that it underlies the concepts of energy bands, the effects of doping on semiconductors, the theory of conductivity, the nature of electron and hole statistics, and many other aspects of semiconductor and device physics. The ultimate equations that we use to describe circuits, such as Ohm's law, or Shockley's equation, are deterministic and classical. Quantum mechanics provides the microscopic basis for these equations, and fixes the parameters appearing in them. To *use* these equations, however, one only needs to know the meaning of the terms which appear in them, and the scope of their applicability.

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In this introductory section we will describe what a quantum computer is. In Sec. 2, we shall describe the ion-trap quantum computer proposed by Cirac and Zoller[3], and summarise the results of an earlier calculation[4] of the decoherence time in this device. An approximate account of this calculation, less technical than that in Ref. [4] is given in an Appendix, along with some details about the structure of the ion array in the trap. Since many reviews of quantum computers now exist,[5] this introductory section may well be redundant for many readers. Readers who are unfamiliar with the subject or with the terms used to describe the contents of the rest of the paper may, however, profit from it.

1.1 What is a Quantum Computer?

The key point is that the state of a classical computer is definite at all times. This is the prevailing rule in classical mechanics. In quantum mechanics by contrast, the state of a physical system is not definite, and a system does not have definite properties until they are measured. The well known uncertainty principle, which expresses the impossibility of simultaneously knowing both the momentum and the position of a particle with definiteness, i.e., with zero uncertainty, is an expression of this fact. In general, therefore, the state of a quantum system must be expressed as a linear superposition of some basis states. Time evolution preserves this superposition property, and since it also conserves probability, must be described by a unitary operator, as long as the system is not externally disturbed.

To understand how these ideas can be usefully applied to make a computer, it is best to take a simple example, that of evaluation of an integer valued function of an integer argument. The first point has to do with the correspondence between numbers and physical states. Thus a single bit (0 or 1) is represented by a physical system or register which can exist in two states, which are represented by $|0\rangle$ and $|1\rangle$. (There are many examples of a two-state system of which we mention only two: the spin of a particle of spin-1/2, and the electronic states of an atom or ion. In the latter case, there are un general many more than two states, and the two-state description is only an approximation. One must be careful to avoid perturbations which will excite the atom or ion into other states.) The novel aspect of a quantum system is that where a classical bit must either be a 0 or a 1, a quantum bit can be any suerposition

$$|\psi\rangle = C_0|0\rangle + C_1|1\rangle, \quad (1)$$

where C_0 and C_1 are arbitrary complex numbers, subject to a normalization condition such as $|C_0|^2 + |C_1|^2 = 1$, expressing the fact that the system has unit total probability for being in some state or other. (We shall leave this normalization out below. This keeps the formulas looking neat, and it is easy to reimpose at any point in the argument.)

The state (1) has no classical interpretation. In particular it is simply incorrect to say that the system *is* in one of the states $|0\rangle$ or $|1\rangle$ with certain probabilities, in the way that we can say that a coin which we toss with our eyes closed *is* either heads or tails even though we don't know exactly which one it is. Such an interpretation of the state leads to wrong predictions for the outcome of many measurements. Similarly, saying that the system is simultaneously in states $|0\rangle$ and $|1\rangle$ has only limited usefulness. One simply has to accept (1) as the state of the system, and use the quantum mechanical assignment of measurables to operators to make predictions.

Next, let us consider a quantum register composed of two two-state systems. The states of this register can be written as $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. Here $|10\rangle$ means that the first two state system is in state 1 and the second in state 0. These four states can be regarded as representations of the four binary numbers 00, 01, 10, and 11. Again, as in Eq. (1), our two two-state-system register can be in a superposition

$$|\psi\rangle = C_{00}|00\rangle + C_{01}|01\rangle + C_{10}|10\rangle + C_{11}|11\rangle. \quad (2)$$

Generalizing to a register of N two-state systems, it is obvious that one can represent 2^N numbers in this way. The general superposition can now be written as

$$|\psi\rangle = \sum_{n=0}^{2^N-1} C_n|n\rangle, \quad (3)$$

where we use the notation $|n\rangle$ to represent a state in which the binary representation of the number n yields the individual state of each two-state system.

Suppose now that we wish to evaluate an integer valued function $f(n)$ of the integers. (We suppose that both n and $f(n)$ are bounded so that we can represent them with registers of manageable size.) Let us assume that we have found a means of dynamically evolving our system in such a way that the corresponding unitary operator U_f transforms the state $|n\rangle$ into $|f(n)\rangle$. More precisely, it is necessary to consider a computer with two registers, which we call the input and the output. The initial state of our computer is taken to be

$$|\psi\rangle_{\text{initial}} = |n\rangle_{\text{in}}|0\rangle_{\text{out}}. \quad (4)$$

Then the unitary operator U_f is supposed to be such that

$$|\psi\rangle_{\text{final}} = U_f|\psi\rangle_{\text{initial}} = |n\rangle_{\text{in}}|f(n)\rangle_{\text{out}}. \quad (5)$$

Note that the input register is left unchanged, while the output register contains the value of the function. Whether or not the operator U_f can be constructed depends on the function f under consideration, and is a separate question, belonging to the theory of algorithms and computability.

The core concept in quantum computing is to take advantage of the superposition principle. It follows from the linearity of the unitary time evolution operator U_f that

$$U_f \sum_n C_n |n\rangle_{\text{in}}|0\rangle_{\text{out}} = \sum_n C_n |n\rangle_{\text{in}}|f(n)\rangle_{\text{out}}. \quad (6)$$

Equation (6) contains the essence of quantum parallelism. Since the effort required to create or implement the evolution U_f is separate and independent of the state of the quantum computer, it follows that if we can prepare the initial state of the quantum computer in the superposition on the left hand side of Eq. (6), the final state will contain, albeit as a superposition, the function $f(n)$ for *all* values of n . We have performed, at first sight, 2^N function evaluations at one shot.

1.2 The Read-Out Problem and Shor's Breakthrough

The parallelism of Eq. (6) is somewhat hollow, however. To obtain information on the function values $f(n)$, one must measure the state of the input and output registers. Such a measurement can only yield *one* value of $f(n)$. We have no way of knowing the other function values. Worse, the value of n for which the function is evaluated is itself random: the probability of getting n is $|C_n|^2$. Thus one could not even generate a table of $f(n)$ by repeated runs of our machine without substantial redundancy.

The above difficulty, also known as the read-out problem, stymied the subject of quantum computers for the decade after its genesis. Interest in the field was primarily in terms of the theory of computability and complexity,[6, 7] and the thermodynamics of computation, specifically the issues of reversibility and energy consumption.[8, 9] The breakthrough came in 1994 with the discovery by Coppersmith and Shor of a quantum algorithm for factorization of a composite number with two prime factors.[10, 11] The key realization is that for certain problems what one needs is not the individual function values $f(n)$, but some global property of the function. In the factorization problem, the property which is exploited is the period of a periodic function. This can be found using Coppersmith's quantum Fourier transform.[10] We refer readers to a recent review of the number theory underlying these algorithms,[12] but briefly and heuristically speaking, quantum mechanics is intrinsically well set up for the efficient addition of terms multiplied by phase factors required in finding a Fourier transform. (Witness the closely related examples of Fraunhofer and N -slit diffraction in optics.) In this way, one can indeed exploit quantum parallelism to do certain calculations very effectively on a quantum computer. For a number with L decimal digits, Shor's algorithm factorizes it in order L^3 steps.¹ The best currently known classical algorithms, by contrast, require

¹For completeness, it should be noted that Shor's algorithm is probabilistic, in that it requires choosing a random number for its operation. The number theoretic method employed by the algorithm fails to give a useful result for certain choices of this random number. However, it can be shown that the probability of success can be made to approach arbitrarily close to unity with $O(L)$ choices of the random number. Thus this consideration does not alter the polynomial time nature of Shor's method.

Table 1: Truth Table for the Controlled-Not Gate

Input	Output
$ 0\ 0\rangle$	$ 0\ 0\rangle$
$ 0\ 1\rangle$	$ 0\ 1\rangle$
$ 1\ 0\rangle$	$ 1\ 1\rangle$
$ 1\ 1\rangle$	$ 1\ 0\rangle$

$\sim \exp[cL^{1/3}(\ln L)^{2/3}]$ steps, where c is a constant of order unity. Needless to say, this discovery has galvanized the subject. The difficulty of factorization is the basis for much modern day cryptography, and the elimination of this difficulty would have obvious repurcussions. In addition, it has been surmised that a generic quantum computer may be used for the simulation of a general many body quantum mechanical problem.[5]

1.3 Primitive Quantum Gates

It remains to say something about how the unitary operator U_f is to be constructed. One would like to do so by composing a small number of basic or primitive operations operating on a small number of bits at a time. Indeed, a one-bit gate consisting of a rotation, and a two-bit gate called the controlled-not (or C-NOT) suffice to build any operator U_f , in the same way that an AND and a NOT suffice for a classical computer. (Equivalently, one could say that any unitary matrix acting on an n dimensional space can be built by multiplying $n(n - 1)/2$ unitary matrices that act on two-dimensional subspaces at a time. The general point that such simple operations can be composed to form arbitrarily complex operators is obvious to any one who has ever solved linear equations by Gaussian elimination or solved matrix problems numerically, but readers who wish to see this codified as theorems should consult Refs. [6, 13, 14, 15]. The physical point which is important is that it is necessary to have a means of introducing correlations amongst the states of two different two-state systems, and this is done via the controlled-not. Any other two-bit gate that was not too close to the identity operation would work just as well.) The one-bit rotate acts on a single bit as follows:

$$U(\phi)(C_0|0\rangle + C_1|1\rangle) = (C_0 \cos \phi + C_1 \sin \phi)|0\rangle + (-C_0 \sin \phi + C_1 \cos \phi)|1\rangle, \quad (7)$$

while the C-NOT acts on any pair of bits as per the truth table in Table 1. The action of this gate is best described in words. It leaves the first (or control) bit unchanged, while the second (or target) bit is flipped from 1 to 0 or vice versa if the control bit is a 1, and left unchanged if the control bit is a 0. It should of course be remembered that this operation also acts on linear superpositions. Thus,

$$a|0\ 1\rangle + b|1\ 1\rangle \xrightarrow{\text{C-NOT}} a|0\ 1\rangle + b|1\ 0\rangle. \quad (8)$$

It should be noted in this connection that the C-NOT is defined with respect to a very definite choice of basis states, which is referred to as the computational basis. It should also be noted that in practical implementations, it may be more useful to construct a few more gates than just the C-NOT and the one-bit rotate. Examples of such gates and simple circuits like adders and multipliers may be found in Refs. [2, 5].

The above discussion of the construction of the evolution operator U_f is very general, and does not say how the individual gate operations are to be carried out. There are at least two broadly different types of quantum computers that have been discussed in the literature. In Feynman's original conception[2], the idea is akin to having an array of sites between which an electron can move, and to arrange the terms in the Hamiltonian to be such that matrix elements between different sites implement the desired gates. It is important that the connections be local in order that the gates remain simple. A computation then proceeds in analogy with an electron wave packet coursing

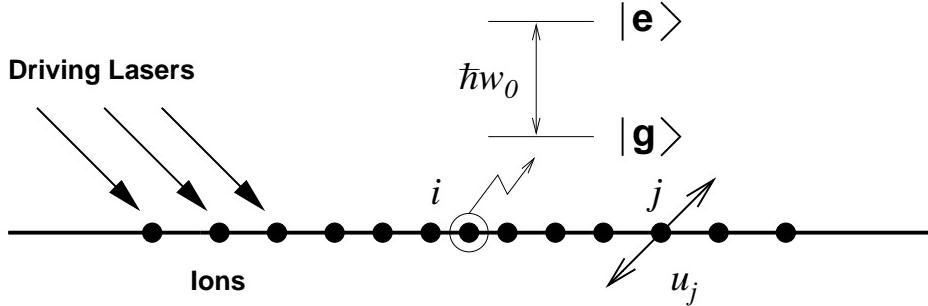


Figure 1: Schematic of the ion-trap quantum computer.

through the sites. The second conception, which is the one more commonly discussed today is to have a temporal sequence of gate operations applied through external perturbations to a fixed set of quantum bits.

With this somewhat long preamble, we now turn to the physical implementation of a quantum computer, especially that based on ion traps.

2 THE ION-TRAP QUANTUM COMPUTER

The desiderata in making a real quantum computer are almost too obvious to state. One needs first and foremost to have a means of controlling and driving the bits individually. Secondly, one needs to have low dissipation, or interaction with the environment. Equation (6) assumes that the computer forms a closed system, isolated from the rest of the world. In reality, interactions with the environment will end up entangling the state of the computer with that of the environment. These interactions are most likely to be such that the correlations amongst the computational degrees of freedom (or quantum bits) get lost over time. This point is well known from the study of problems like NMR, where also one has many quantum systems, each with a Hilbert space of small dimensionality, but interacting with an environment — the lattice, motional degrees of freedom of the atoms, electromagnetic radiation, etc.

Even after the above conditions are met, it is not easy to implement a good two-bit gate. In addition to the ion-trap proposal[3] that we shall describe in more detail, another one based on cavity QED[16] seems promising. In fact, experimental two-bit gates, inspired by each of these schemes, were demonstrated shortly after their proposal.[17, 18]

The ion-trap QC utilizes an array of N identical ions in a linear rf Paul trap, each of which can be independently addressed and driven by a laser. (See Fig. 1.) The ions are cooled to nearly zero temperature. Such arrays have been studied for some time now because of the opportunities they offer for spectroscopy, and developing frequency standards.[19, 20] The ions have a nonuniform spacing determined by the Coulomb repulsion between the ions and the effective trap potential. A quantum bit is composed of two internal states of an ion, which we denote by $|e\rangle$ and $|g\rangle$, and one-bit gates are executed by applying suitable pulses ($\pi/2$, π , etc.) to the ions. The clever idea which enables the execution of a two-bit gate is to use the center of mass motion of the entire array as an additional computational degree of freedom. Let ω_0 be the $g \leftrightarrow e$ transition frequency of the ions, and let ω_z be the center of mass vibrational frequency. A laser pulse with carrier frequency $\omega_0 \pm \omega_z$ acting on the i th ion entangles the internal state of this ion with that of the center of mass mode. As discussed in Ref. [3], a sequence of three such pulses, the first and third applied to ion i , and the second to ion j , have the net effect of a two-bit gate in which ions i and j are the control and target bit, respectively. In fact, by also applying one-bit rotate operations to ion j , this gate can be exactly turned into the C-NOT. A sequence of one- and two-bit gate operations can then be executed, yielding any desired computation, as discussed in Sec. 1.

2.1 Spontaneous Emission Decoherence

The advantages of the ion-trap QC are its conceptual simplicity, and high degree of isolation from the environment. In fact, the proposal is regarded seriously enough that an effort is underway to build a proof-of-principle prototype.[21] The most obvious source of decoherence is the spontaneous emission from the ions. It seems reasonable that effects like superradiance, in which the proximity of the ions to one another affects this decay, can be neglected, and that each ion can be treated separately. If we assume that half the ions are in an excited state at any given time on the average, then in a computer with N ions, any computation must be completed in a time of order $\tau_{\text{rad}} = 2\tau_s/N$, since even one spontaneous emission event destroys the phase coherence among the computational basis states of the QC as a whole. One can minimize this source of decoherence by employing ions where the $|e\rangle$ state can not decay to any state other than $|g\rangle$ and the decay in question is dipole forbidden. For example, in Ba^+ ions, the decay between the $5d\ ^2D_{5/2}$ multiplet (one member of which serves as $|e\rangle$) and the $6s\ ^2S_{1/2}$ multiplet (which supplies the $|g\rangle$ state) is via an E2 process, for which $\tau_s = 30\text{-}70$ s.² The drawback, as noted by Plenio and Knight[22] is, that by the general relation between Einstein A and B coefficients, the coupling of the laser to the $g \leftrightarrow e$ transition is also weak, and the time required for all gates is correspondingly long. One can not shorten this time without limit by increasing the laser power without starting to excite the ion into higher levels, or even ionize it further, via two-photon absorption. The radiative decoherence can be decreased by working with a Λ system and using Raman pulses, but it can not be totally eliminated.[22]

2.2 Vibrational Decoherence

The second source of decoherence in the ion-trap QC is the ionic vibration. To understand this, suppose (see Fig. 1), ion j is displaced from its equilibrium position. This creates an excess electric field or electric field gradient at any other ion, say i . The time evolution in the $|e\rangle$, $|g\rangle$ space of ion i is thereby altered, and in the long run, the QC is not in the intended state, i.e., we have decoherence. Let us denote the decoherence time due to this process by τ_{vib} . A proper calculation of this time is not so easy as that of τ_{rad} as all the ions are coupled to the same bath, and can not be treated individually. A naive consideration based on only a few ions leads to an overestimate, and is misleading. The calculation presented in the Appendix shows that τ_{vib}^{-1} scales more rapidly than N , where N is the number of ions. More precisely, we find,

$$\tau_{\text{vib}}^{-1} \sim N^{1/2} \frac{q^2 Q^2}{2\pi\hbar m\omega_0\omega_t s_0^8}, \quad (9)$$

where Q is a quadrupole transition matrix element (appropriate to the Ba^+ example), ω_t is a typical transverse normal mode frequency for the ion array, q and m are the ionic charge and mass, and s_0 is the minimum spacing between the ions which occurs at the center of the array. We can write τ_{vib}^{-1} more explicitly as a rate by noting that $q^2 = m\omega_z^2 d_0^3$, where d_0 is the trap length scale parameter [see Eq. (34)], and that

$$Q^2 \propto \hbar/\tau_s k_0^5, \quad (10)$$

where $k_0 = \omega_0/c$. It follows that

$$\frac{1}{\tau_{\text{vib}}} \sim \frac{N^{1/2}}{\tau_s} \left(\frac{d_0}{s_0} \right)^3 \frac{\omega_z^2}{\omega_0 \omega_t} \frac{1}{(k_0 s_0)^5}. \quad (11)$$

2.3 Discussion of Results

Equation (11) has interesting implications for the scaling of τ_{vib} with N . We can not naively take this as $N^{1/2}$ because the behaviour of ω_z , ω_t , and s_0 as N is increased, depends on how the trap operating conditions are varied. Suppose s_0 is held fixed as N is increased. Then $(d_0/s_0)^3 \sim N^2/\ln N$ and $\tau_{\text{vib}}^{-1} \sim N^{5/2}/\ln N$. In this case, however, the longitudinal voltage on the trap electrodes, which is

²Other ions in groups IIA and IIB, such as Ca^+ and Hg^+ , have similar level schemes, and long spontaneous decay times.

proportional to ω_z^2 , varies as $(\ln N)/N^2$. Since the time needed for a two-bit gate varies as ω_z^{-1} , the total computational time goes up. Secondly, the longitudinal confinement becomes weaker, and non-linearities in the trapping potential, and electrode patch voltages become more important. Suppose, on the other hand, that the trap voltages, and therefore, ω_z and ω_t , are held fixed as N increases. Then $\tau_{\text{vib}}^{-1} \sim N^{35/6}(\ln N)^{-8/3}$. [The variation is as $N^{9/2}(\ln N)^{-2}$ for an E1 transition.] Now, however, the minimum inter-ion spacing s_0 varies as $\sim N^{-2/3}$. This may make it difficult to optically resolve and address individual ions, which is basic to the operation of the QC. It seems likely that some compromise between these two extremes will have to be sought, depending on engineering considerations. A general point is worth noting in this connection. Since the radiative and vibrational decoherence processes are independent, the total decoherence time of the computer is given by adding their *rates*:

$$t_d = (\tau_{\text{rad}}^{-1} + \tau_{\text{vib}}^{-1})^{-1}. \quad (12)$$

t_d is the useful window of time in which any computation must be finished. Thus if one of the two rates turns out to be much larger than the other, we can relax the design considerations on the smaller rate, and focus on ways to reduce the larger one.

Let us estimate τ_{vib} using the example of Ba^+ ions and the levels mentioned above. The frequency $\omega_0 = (2\pi)1.7 \times 10^{14}$ Hz. We take $\omega_z/2\pi = 100$ kHz, and $\omega_t/2\pi = 20$ MHz. This yields $d_0 = 14 \mu\text{m}$. For $N = 1000$, we obtain $\tau_{\text{vib}} \simeq 10^4 \tau_s$, which is surprisingly large. (It is even larger in comparison to $\tau_{\text{rad}} = \tau_s/N$.) The drawback is that $s_0 \simeq 0.5 \mu\text{m}$ with the same parameters. This runs into the difficulty with optical resolution mentioned above. We have not explored compromise variations of trap parameters in detail.

It is natural to ask if we should not have anticipated τ_{rad} being so much larger than τ_{vib} . The non-trivial scaling with N and the fact that the relationship would reverse for larger N makes us believe that the answer is no.

2.4 Conclusion

In summary, vibrational decoherence is not a significant problem in the ion-trap QC for $N \leq 10^3$, as originally envisaged by Cirac and Zoller.[3] This optimistic result should be tempered somewhat however. The technical difficulties in working with 10^3 ions are enormous, and the spontaneous emission decoherence itself is nothing to sneeze at. It is possible that the Λ system with Raman transitions will mitigate this difficulty, but this needs to be explored more fully. A qualitative argument suggests that the adiabatic suppression of τ_{vib}^{-1} will not be as effective in this case, however. If this turns out to be true, it would provide a nice example of the compromise between different types of decoherence discussed above.

A CALCULATION OF VIBRATIONAL DECOHERENCE TIME

We give here an approximate calculation of the vibrational decay time. The calculation is based on Ref. [4] which should be consulted for a more precise description.

We denote the equilibrium axial position of the j th ion by z_j , and its deviation from equilibrium by \mathbf{u}_j . We will consider a $g \leftrightarrow e$ transition of electric quadrupole (E2) type, and denote the ionic charge by q , and the quadrupole transition matrix element by Q , ignoring all vector and tensor indices, here and in what follows. The coupling between the vibrations and the eg space of the i th ion is described the Hamiltonian

$$V_i = \sum_{j \neq i} \frac{qQ}{|z_i - z_j|^4} u_j (|e\rangle\langle j| + \text{h.c.}). \quad (13)$$

The effect of this perturbation is small for two reasons. First, its magnitude is small, $|V_i| \ll \hbar\omega_0$. Second, the time scale for its variation is determined by the ion array's normal mode frequencies,

which are of order 100 MHz at most, and thus much less than ω_0 , which is an optical transition frequency of order 100 THz or more. Formally,

$$\left| \frac{\dot{V}_i}{V_i} \right| \ll \omega_0. \quad (14)$$

The perturbation is thus slow, and the internal state of the ions can follow the vibrational disturbances adiabatically. If this following were perfect, we would have no real excitations or transfer of energy. Decoherence arises solely because of corrections to the adiabatic approximation, and we can thus expect the final answer for τ_{vib}^{-1} to contain a small factor like $(\omega_v/\omega_0)^a$ where a is a positive exponent, and ω_v is a typical vibrational time. We now turn to estimating this effect.

A.1 Adiabatic Approximation

Let us map each two-state ion onto an equivalent spin-1/2 system, with $|e\rangle$ and $|g\rangle$ being the up and down spin states. The i th spin sees effective magnetic fields $B_z = \hbar\omega_0$ and $B_\perp(t) = V_i(t)$ (see Fig. 2), where we take $V_i(t)$ to be a specified time dependent c-number perturbation. The total Hamiltonian for this ion can thus be written as

$$\mathcal{H}_i = \frac{1}{2}\hbar\omega_0\sigma_z + \hbar\mathbf{f}(t) \cdot \vec{\sigma}, \quad (15)$$

where $\mathbf{f}(t) = (B_x, B_y, 0)/2\hbar$, and the σ 's are the usual Pauli matrices in the equivalent spin space. Note that \mathbf{f} has no z component.

We wish to study the time evolution of the spin for a general $\mathbf{f}(t)$ which is small and slow. To this end, let us write a general spin state as

$$|\psi(t)\rangle = u_+(t)e^{-i\omega_0 t/2}|+\rangle + u_-(t)e^{i\omega_0 t/2}|-\rangle. \quad (16)$$

where $|\pm\rangle$ denotes the eigenstates of S_z with eigenvalues $\pm 1/2$. Schrödinger's equation gives

$$i\dot{u}_\pm = e^{\pm i\omega_0 t} f_\mp(t) u_\mp(t), \quad (17)$$

where $f_\pm = f_x \pm if_y$. Since f_\pm varies very slowly, we try a solution to Eq. (17) of the form

$$u_\pm(t) = \alpha_\pm(t) + \beta_\pm(t), \quad (18)$$

where α_\pm and β_\pm are functions that vary rapidly and slowly, respectively. The latter is almost a constant over a period $2\pi/\omega_0$, and the former almost averages to zero.

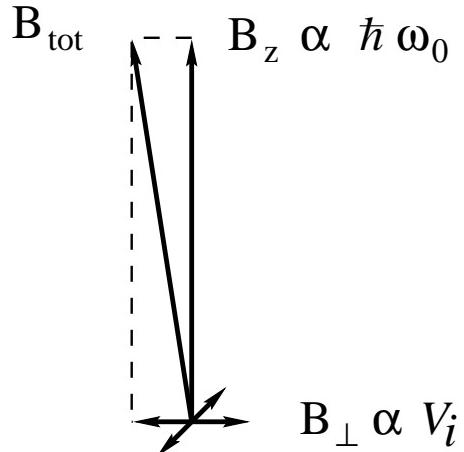


Figure 2: Equivalent magnetic field description of i th ion.

We now substitute Eq. (18) in Eq. (17), and separately equate the fast and slowly varying parts. This yields

$$i\dot{\alpha}_{\pm} = e^{\pm i\omega_0 t} f_{\mp}(t) \beta_{\mp}(t), \quad (19)$$

$$i\dot{\beta}_{\pm} = e^{\pm i\omega_0 t} f_{\mp}(t) \alpha_{\mp}(t). \quad (20)$$

The next step is to integrate these equations. Consider Eq. (19) first. To a first approximation, we can regard f_{\pm} and β_{\pm} as constants. Integration then gives

$$\alpha_{\pm} = \mp \omega_0^{-1} e^{\pm i\omega_0 t} f_{\mp}(t) \beta_{\mp}(t). \quad (21)$$

Substitution of this result in Eq. (20) yields

$$i\dot{\beta}_{\pm} = \pm \frac{|\mathbf{f}(t)|^2}{\omega_0} \beta_{\pm}(t). \quad (22)$$

Integrating this equation, we obtain

$$\beta_{\pm}(t) = \exp(\mp i\Phi(t)) \beta_{\pm}(0), \quad (23)$$

where

$$\Phi(t) = \int_0^t dt' \frac{|\mathbf{f}(t')|^2}{\omega_0}. \quad (24)$$

We next note that since by Eq. (21), $|\alpha_{\pm}/\beta_{\pm}| \approx |f_{\pm}/\omega_0| \ll 1$, $u_{\pm} \approx \beta_{\pm}$ in leading order in f_{\pm}/ω_0 . Equations (23), (24), and (16) thus give us the desired expression for the time dependence of a general state.

The above equations also give us the amount of decoherence. Suppose the initial state of the spin is $2^{-1/2}(|+\rangle + |-\rangle)$, i.e., $u_{\pm}(0) = 2^{-1/2}$. (A product of states of this type for each quantum bit is the starting point in several quantum algorithms.) Let the state that would be obtained at time t in the absence of the perturbation \mathbf{f} be $|\psi_0(t)\rangle$. The states $|\psi_0(t)\rangle$ and $|\psi(t)\rangle$ are the states of the quantum bit in the ideal and actual QC, without and with decoherence. The decoherence is given by the overlap

$$\langle \psi_0(t) | \psi(t) \rangle = \cos(\Phi(t)). \quad (25)$$

Another way to understand these results is that because $|B_{\perp}| \ll B_z$, the precession axis for the spin can be taken to be $\hat{\mathbf{z}}$ at all times to very good approximation, and the instantaneous precession frequency can be taken as

$$\omega'_{0i} = (\omega_0^2 + V_i^2/\hbar^2)^{1/2} \approx \omega_0 + \frac{V_i^2}{2\hbar^2\omega_0}. \quad (26)$$

Hence, the time dependence of the states $|\pm\rangle$ is given by $\exp\left(\pm i \int_0^t dt' \omega'_{0i}(t')/2\right) |\pm\rangle$. [Note that $\Phi(t)$ is just half the difference between $\int_0^t \omega'_{0i}(t') dt'$ and ω_{0i} .]

A.2 Single and Many Ion Decoherence Times

The decoherence time for the i th ion is approximately equal to the time required for its phase to deviate from its unperturbed value by π : $\tau_i \approx \pi/(\omega'_{0i} - \omega_0)$. Using Eqs. (13) and (26), we obtain

$$\tau_i^{-1} \approx \frac{q^2 Q^2}{2\pi\hbar^2\omega_0} \left\langle \left(\sum_{j \neq i} \frac{u_j}{(z_i - z_j)^4} \right)^2 \right\rangle, \quad (27)$$

where the angular brackets denote some kind of average. In principle this average should be calculated by expressing the displacements \mathbf{u} in terms of the normal modes of the array, which should be described by a thermal density matrix at the temperature T to which they have been cooled. (Additional correlations from the center of mass mode excitations inherent in the two-bit gates should be excluded since they are part of the intended time evolution and do not generate decoherence.)

We have already left this part out in deriving Eq. (27) by taking \mathbf{f} to be slow.) We are interested in obtaining an order of magnitude answer. Therefore, we will ignore the normal mode structure, and assume each ion to vibrate independently with some average frequency. Secondly, to obtain the best-case answer, we will assume that $T \ll \hbar\omega_z/k_B$, and simply set $T = 0$. To be more concrete, we write

$$\langle u_j u_k \rangle = \frac{\hbar}{m\omega_t} \delta_{jk}, \quad (28)$$

where ω_t is a typical transverse mode frequency, and m is the ionic mass. It follows that

$$\tau_i^{-1} \approx \frac{q^2 Q^2}{2\pi\hbar m\omega_0\omega_t} \sum_{j \neq i} \frac{1}{(z_i - z_j)^8}. \quad (29)$$

There are two reasons for using a transverse mode frequency in Eq. (28). First, in the linear Paul trap, these frequencies are generally higher than the longitudinal ones. Second, one can arrange via a J_z selection rule for the longitudinal modes not to excite any $g \leftrightarrow e$ transitions.

We now combine the individual ion decoherence times to obtain τ_{vib} for the QC as a whole. The obvious procedure of adding the rates is not quite correct. The reason can be seen from Eq. (25). The overlap between the actual and intended states of the i th spin is more like $\cos(t/\tau_i)$ than $\exp(-t/\tau_i)$. Multiplying these overlaps for all spins, we obtain $P(t) \simeq \prod_i \cos^2(t/\tau_i) \simeq \exp(-t^2/\tau_{\text{vib}}^2)$ with

$$\tau_{\text{vib}}^{-2} = \sum_i \tau_i^{-2}. \quad (30)$$

A more careful justification for this result can be found in Ref. [4]. We note here that if we simply add τ_i^{-1} to obtain τ_{vib}^{-1} , we overestimate τ_{vib}^{-1} by a multiplicative factor of $N^{1/2}$; if this were done, the $N^{1/2}$ in Eq. (11) would change to N .

A.3 Continuum Approximation for Ion Array

Equations (29) and (30) provide us with a formal answer for the vibrational decoherence rate. To obtain a more useful result, however, it is necessary to perform the sums over the lattice positions. For small N , say 25 or less, these sums are best done numerically, but for larger N , we can evaluate them by approximating the ion array as a continuum.

Let us define $s(z_i)$ to be the average of the local spacing between the ion at z_i and its two nearest neighbours. We expect that for large N , this spacing will vary slowly as we move along the array. Hence, it is a good approximation to treat z as a continuous variable, and on this basis we will find an expression for $s(z)$. We will also find the total length of the array as a function of N .

Consider an ion at position z , and let us denote the separations to its immediate neighbours to the left and right by s_- and s_+ respectively. The Coulomb force on the ion at z from these near neighbours is given by

$$F_{\text{nn}}^{\text{Coul}} = q^2(s_-^{-2} - s_+^{-2}) \approx 2q^2 s^{-2}(ds/dz), \quad (31)$$

since $s_+ - s_- \approx s(z)(ds/dz)$. For ions not too close to the edge of the array, the distances to the second, third, fourth, neighbour pairs are approximately doubled, tripled, quadrupled and so on. The forces from these successively distant neighbour pairs are smaller than $F_{\text{nn}}^{\text{Coul}}$ by factors of 4, 9, 16, etc. Since, $\sum_{n=1}^{\infty} n^{-2} = \pi^2/6$, and since the sum converges very rapidly, we can write the net Coulomb force on the ion at z as

$$F_{\text{net}}^{\text{Coul}} = (\pi^2 q^2 / 3s^2)(ds/dz). \quad (32)$$

Equating this to the opposing spring force $m\omega_z^2 z$ from the trapping potential, we obtain a differential equation for the spacing function:

$$\frac{\pi^2}{3s^2(z)} \frac{ds}{dz} = \frac{z}{d_0^3}. \quad (33)$$

We have introduced

$$d_0 = (q^2/m\omega_z^2)^{1/3} \quad (34)$$

as a natural length scale for the trap. (One can easily show that the ion spacing is of order d_0 for 2 or 3 ions in the trap.)

To integrate Eq. (33), we define the total length of the array to be $2L$. Choosing the center to be at $z = 0$, we obtain

$$\frac{1}{s(L)} - \frac{1}{s(z)} = -\frac{3}{2\pi^2 d_0^3} (L^2 - z^2). \quad (35)$$

To make use of this result, however, we need expressions for L and $s(L)$. To find $s(L)$, we use same argument as was used to obtain Eq. (32), although the approximation is clearly not as good now. We assume that the spacing between the ions near the end of the chain is uniform and equal to $s(L)$. The Coulomb force on the last ion is then $\pi^2 q^2 / 6s^2(L)$. Balancing this with the spring force $m\omega_z^2$, we obtain $s(L) \approx \pi(d_0^3/6L)^{1/2}$. Even if this argument is not watertight, it shows that we can ignore $s^{-1}(L)$ compared to $3L^2/2\pi^2 d_0^3$ in Eq. (35). This yields

$$s(z) = s_0(1 - z^2/L^2)^{-1}, \quad (36)$$

where we have introduced the minimum ion spacing (attained at $z = 0$):

$$s_0 \equiv s(0) = 2\pi^2 d_0^3/L^2. \quad (37)$$

It still remains to find $L(N)$. If we denote the ion number at position z by $n(z)$, then $dn/dz = 1/s(z)$ in the continuum approximation. Integration of this result along with Eq. (36) gives

$$L = d_0(\pi^2 N/2)^{1/3}, \quad (38)$$

$$s_0 = 6.81d_0N^{-2/3}. \quad (39)$$

One can also show that the mean spacing varies as $N^{-2/3} \ln N$.

The treatment of the ends of the chain above is not fully satisfactory. Another continuum approach is due to Dubin.[23] He regards the array as fluid of total charge qN . It is known that in a harmonic potential such as that of the trap, such a fluid forms an ellipsoid of revolution of uniform charge density. When the trap is much stiffer in the transverse than the longitudinal direction, i.e., $\omega_t \gg \omega_z$, the ellipsoid has a total volume $4\pi N d_0^3$. Equating the semi major axis of the ellipsoid to L , we find the semi minor axis to be $(3Nd_0^3/L)^{1/2}$. The spacing $s(z)$ is now given by geometry. Let $A(z)$ be the cross sectional area of the ellipsoid at an axial distance z from the center. The volume $s(z)A(z)$ clearly contains one unit q of charge, from which it follows that

$$\frac{1}{s(z)} = \frac{3}{4} \frac{N}{L} \left(1 - \frac{z^2}{L^2}\right). \quad (40)$$

This agrees with Eq. (36), but s_0 has a different form. To complete the solution, we must find this form, or equivalently, $L(N)$. The fluid model answer for L depends on ω_z/ω_t , which is clearly wrong if the linear structure is stable. Dubin therefore resorts to a local density functional theory to estimate the discreteness correction to the Coulomb energy. He then minimizes the sum of this correction, the fluid drop self energy, and the trapping potential energy. The resulting array length is independent of ω_z/ω_t and is given by

$$L^3 = 3N \ln(c_0 N) d_0^3, \quad (41)$$

where $c_0 = 6e^{\gamma-13/5} \approx 0.8$, and γ is Euler's constant. We also obtain

$$s_0 = 4L/3N = 1.92N^{-2/3}[\ln(0.8N)]^{1/3}d_0. \quad (42)$$

These results differ from Eqs. (38) and (39) logarithmically in N .

It is interesting to compare these results with some recent semi-numerical work by Meyrath and James.[24] They integrate Eq. (36), write the result as $n(z) = az - bz^3$, and fit a and b to power laws in N instead of trying to relate them to s_0 and L . They then invert this cubic equation for $z(n)$, and find that the answer agrees quite well with numerics for $N \geq 25$. Likewise, Eq. (42) provides a very good fit to the numerical results.

A.4 Lattice Sums

Equations (40-42) can be used to find the sums in Eqs. (29) and (30). The first type of sum,

$$S_n(i) \equiv \sum_{j \neq i} \frac{1}{|z_i - z_j|^n}, \quad (43)$$

can be very simply evaluated as

$$S_n(i) \approx 2s^n(z_i) \sum_{j=1}^{\infty} \frac{1}{j^n} = \frac{2\zeta(n)}{s^n(z_i)}. \quad (44)$$

This result should hold well for all i except very close to the ends, since the exponent n is big (3 for an E1 decay, 4 for E2).

The second type of sum is $T_n = \sum_i s^{-n}(z_i)$. Writing $\Delta i \approx dz/s(z)$, we can approximate it by an integral:

$$T_n = \sum_i \frac{1}{s^n(z_i)} \approx \int_{-L}^L \frac{dz}{s^{n+1}(z)}. \quad (45)$$

Substituting Eq. (36) and performing the integration, we obtain

$$T_n \approx \frac{L}{s_0^{n+1}} \left(\frac{4\pi}{4n+7} \right)^{1/2}, \quad (46)$$

where we have also used an asymptotic formula for $\beta(n+2, 1/2)$.

The combination of Eqs. (44) and (46) with Eqs. (29) and (30) leads to the results (9)-(11) quoted in Sec. 2.

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